# New Methodologies for Analysis of Premixed Charge Compression Ignition Engines

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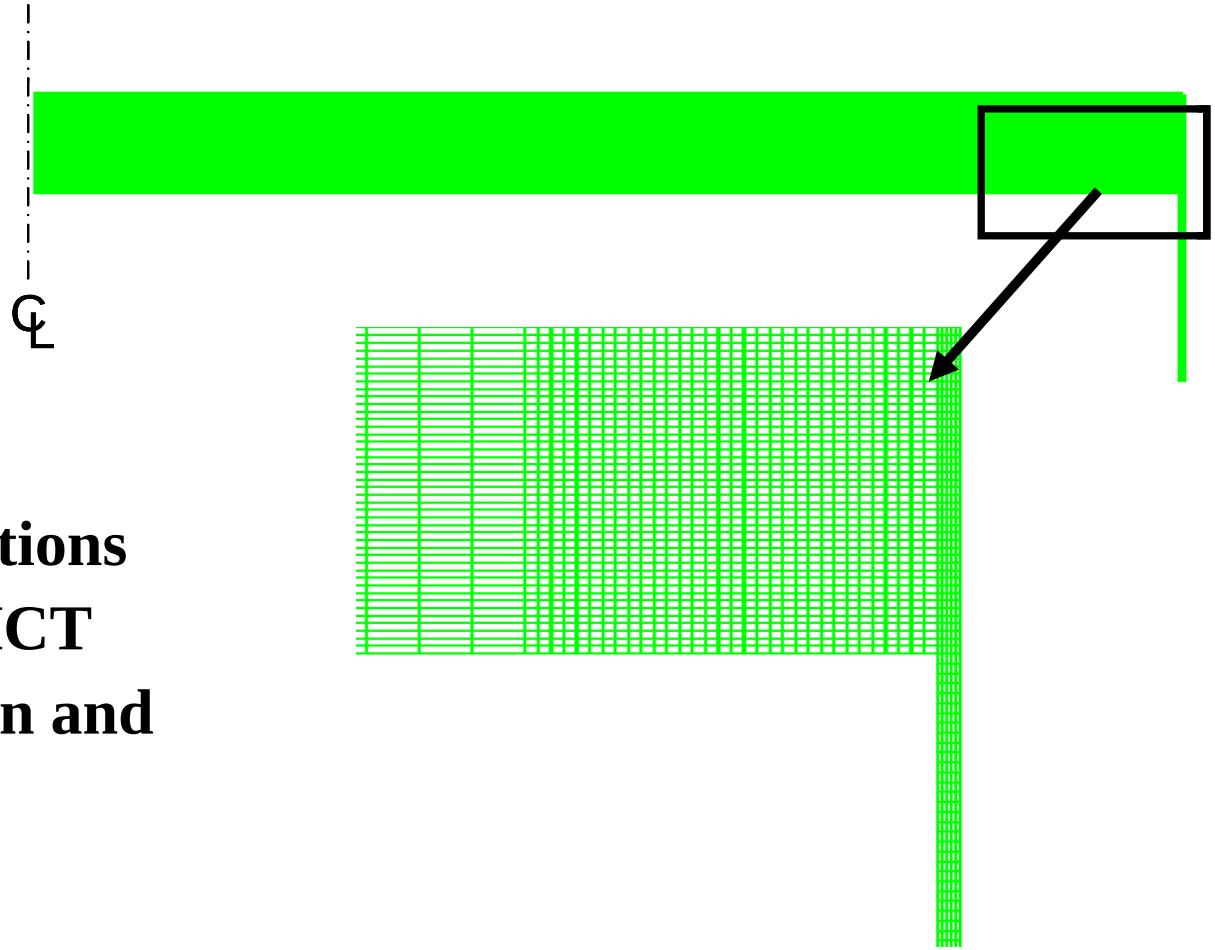
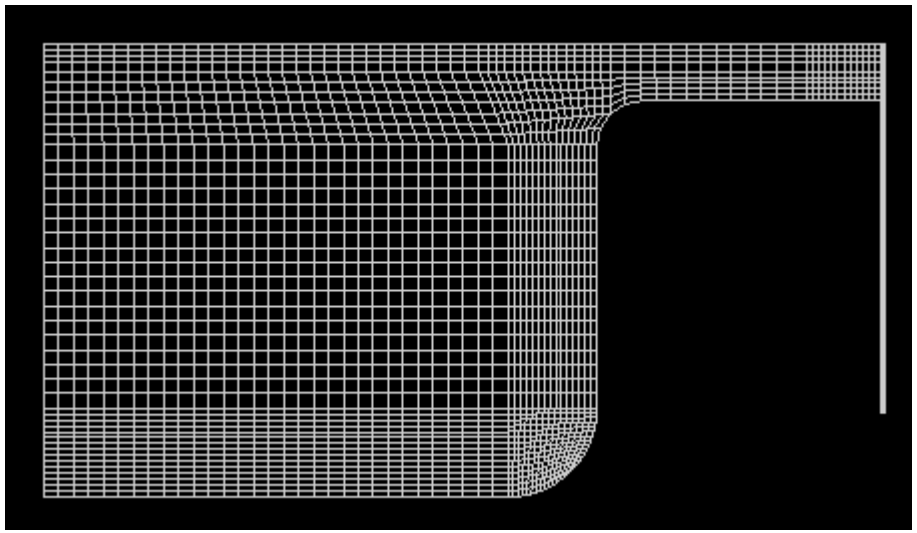
# Engine combustion problems could theoretically be solved by integrating a chemical kinetics and a fluid mechanics code



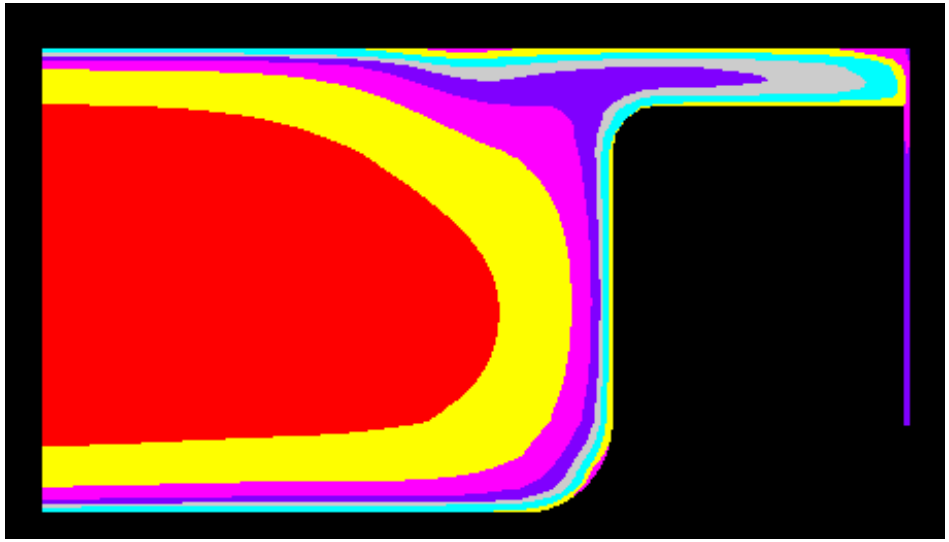
- **KIVA calculates temperature distributions and CHEMKIN or HCT calculates composition and heat release**
- **Appropriate spatial resolution and a detailed mechanism are necessary**

# The physics of HCCI combustion can be well captured with a sequential fluid mechanics-chemical kinetics model

High resolution CFD simulation ($10^5$-$10^6$ cells)



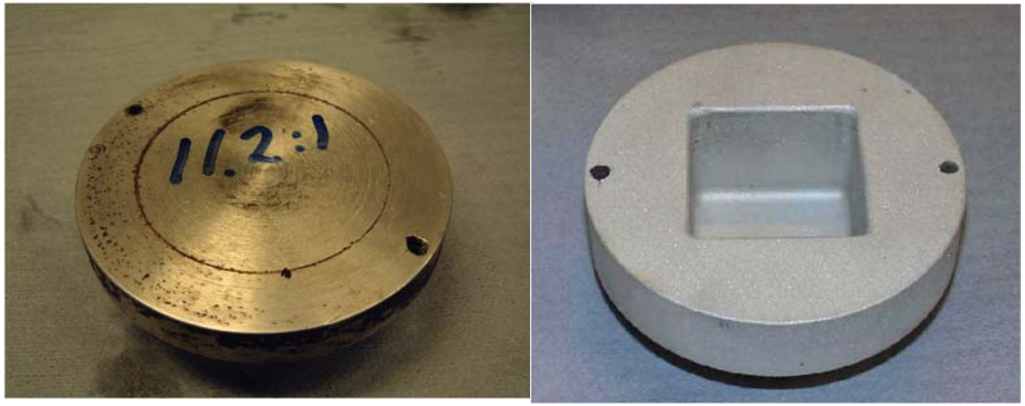
Lower resolution chemical kinetics discretization (10-100 zones)



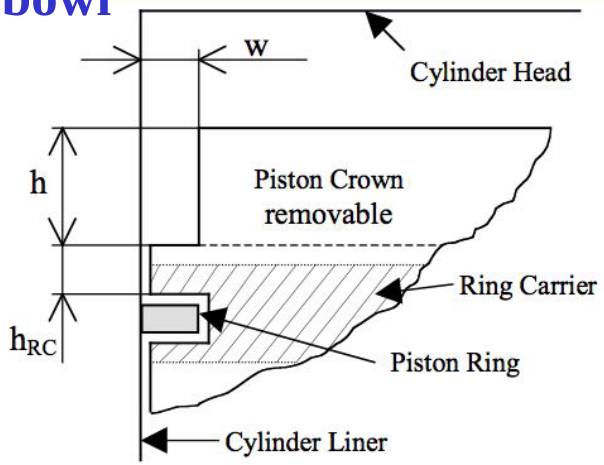
Fluid mechanics sets the temperature distribution where autoignition occurs

Combustion is very fast and therefore can be analyzed without considering mixing or turbulence

# Model has been very successful in predicting HCCI combustion in multiple geometries, fuels, and operating conditions

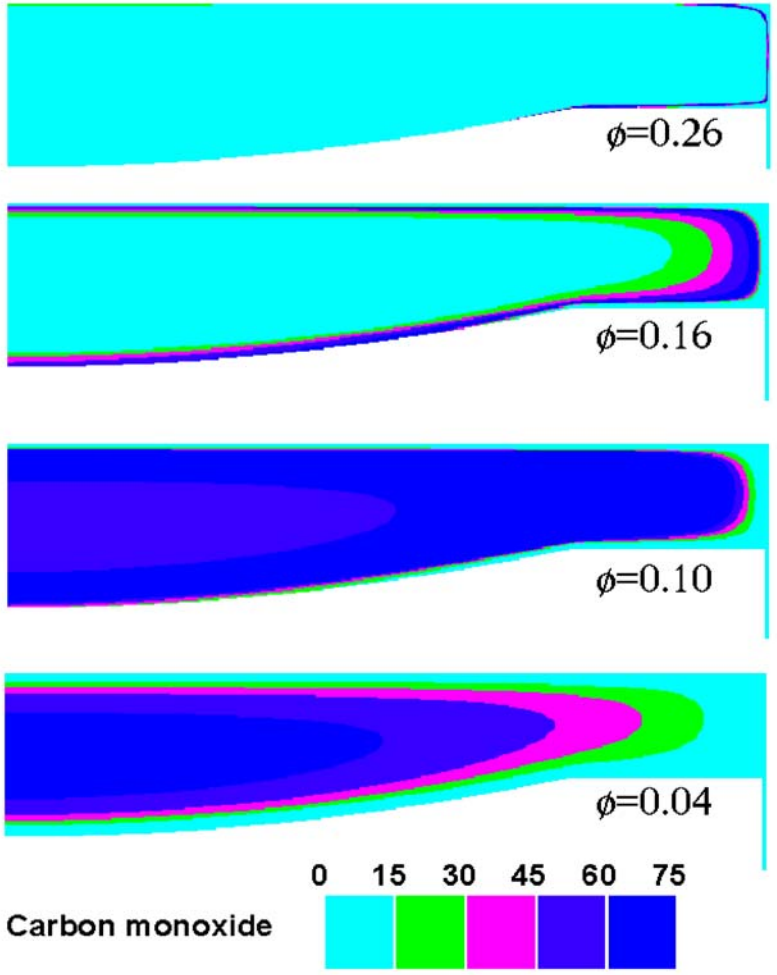



**Combustion is slower with high turbulence square bowl**



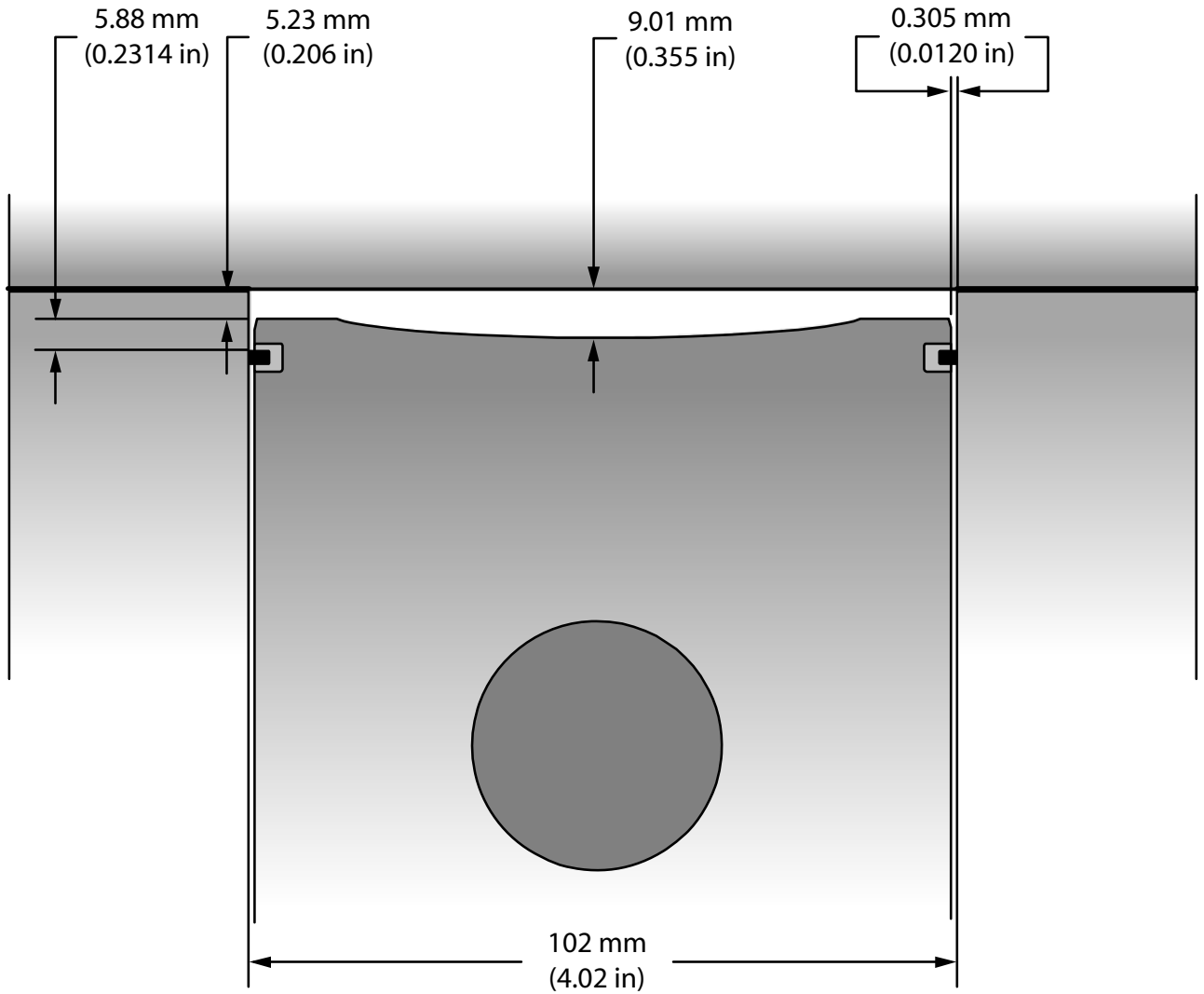

**Crevice width w=0.26 mm, 1.6 mm and 2.1 mm**
**Constant compression ratio 17:1**

**HC emissions are a non-monotonic function of crevice width**

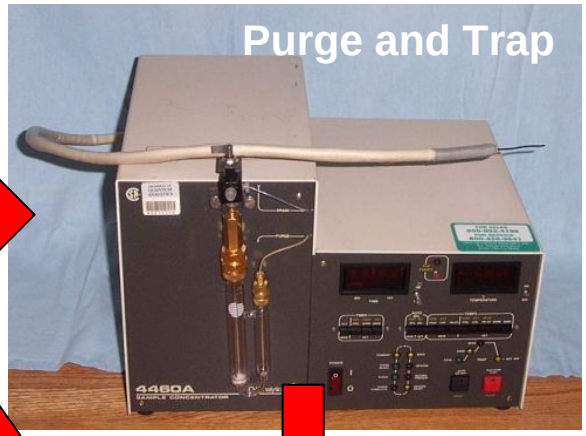



**Combustion chamber locations where CO is produced**

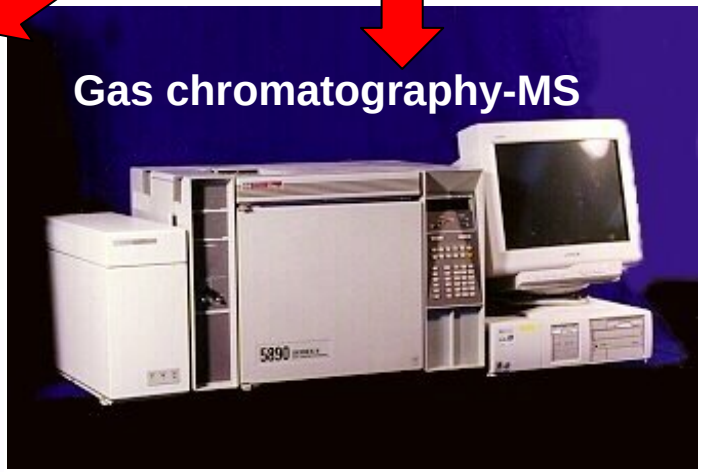
# Problem: Can we predict exhaust composition, down to the small hydrocarbon species?



# Analytical chemistry group at LLNL has measured concentration of 40 intermediate hydrocarbons in Sandia HCCI engine exhaust

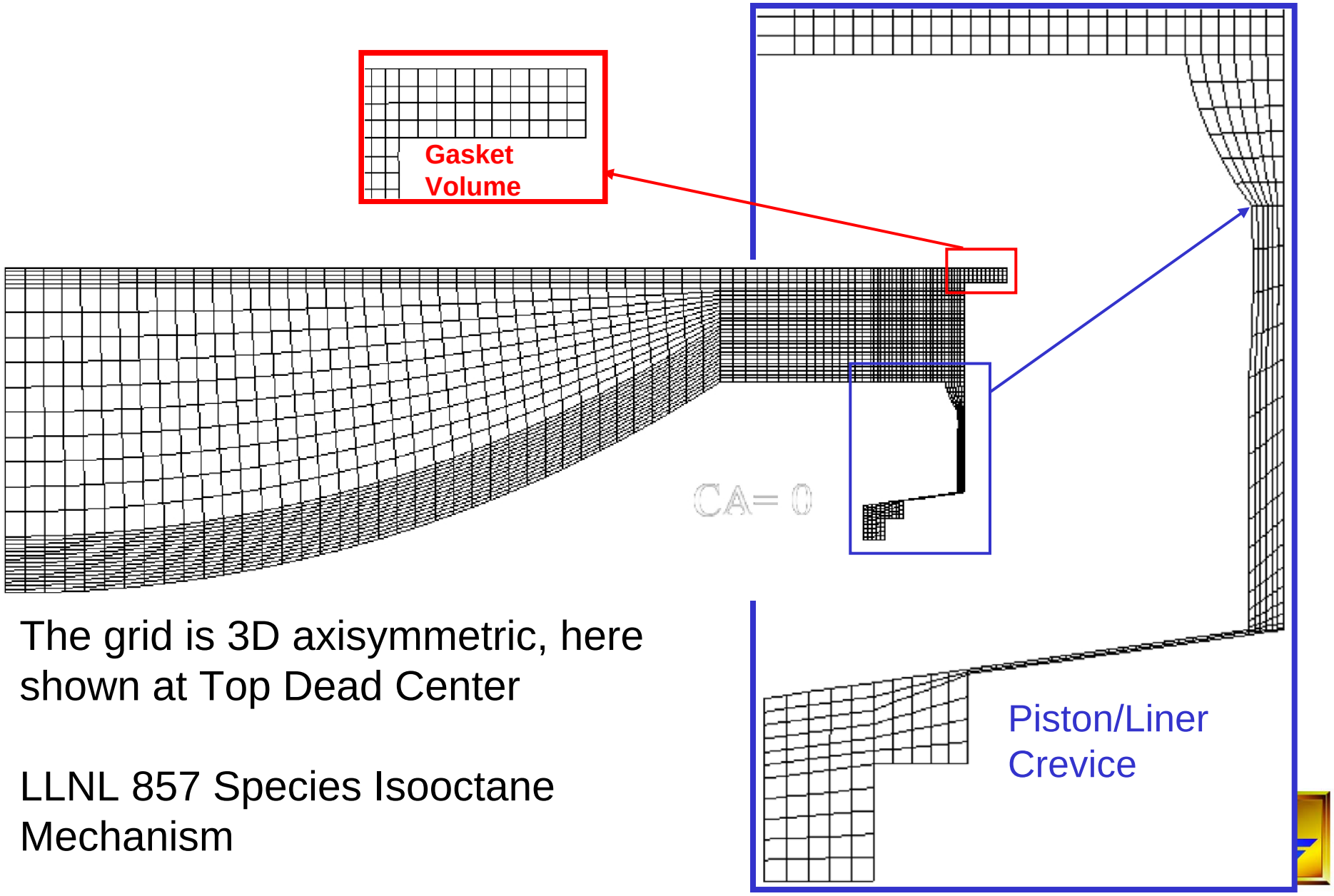




Liquid chromatography




| Authentic Standards |
|---|
| 2-methylbutane |
| formaldehyde |
| acetaldehyde |
| acetone |
| n-butanal |
| 4-methyl-2-pentane |
| 2,2,4-trimethylpentane |
| n-heptane |
| toluene |
| 2,2,5,5-tetramethyltetrahydrofuran |
| n-nonane |

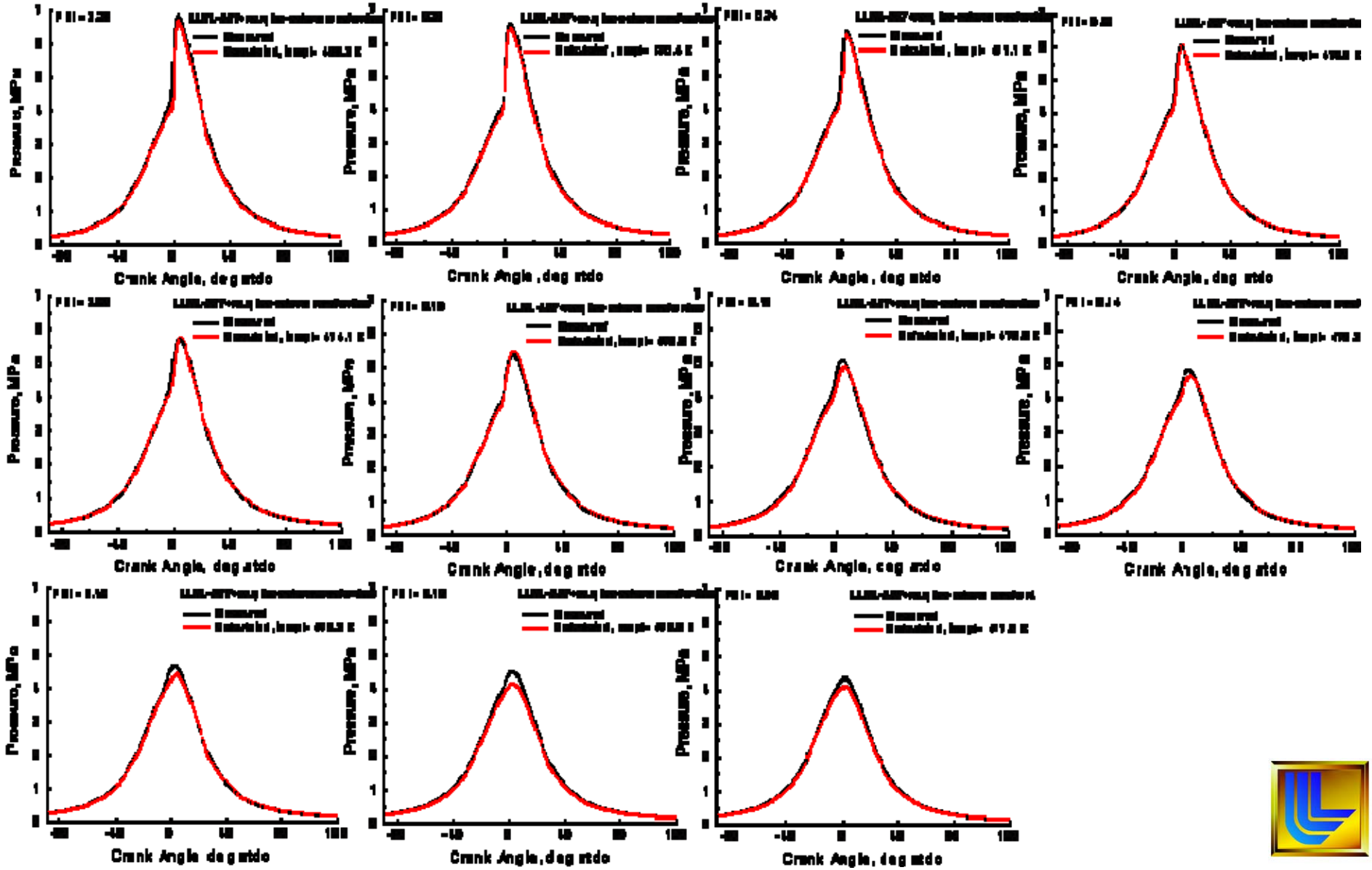
# We have conducted high fidelity analysis of Sandia engine: Our KIVA3V grid resolves the combustion chamber in detail



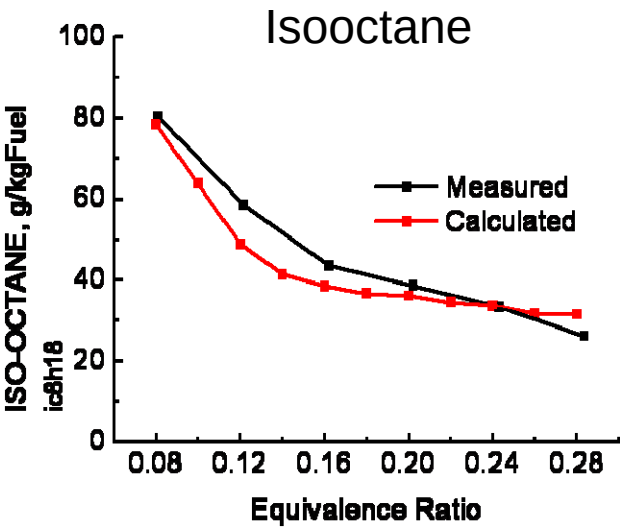

The grid is 3D axisymmetric, here shown at Top Dead Center

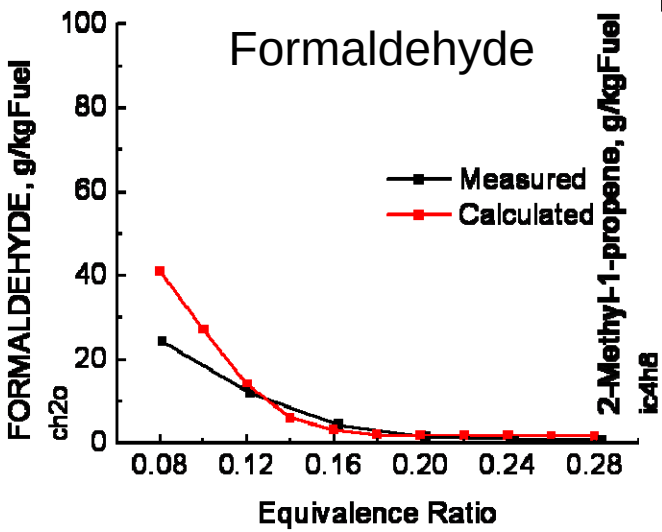
LLNL 857 Species Isooctane Mechanism

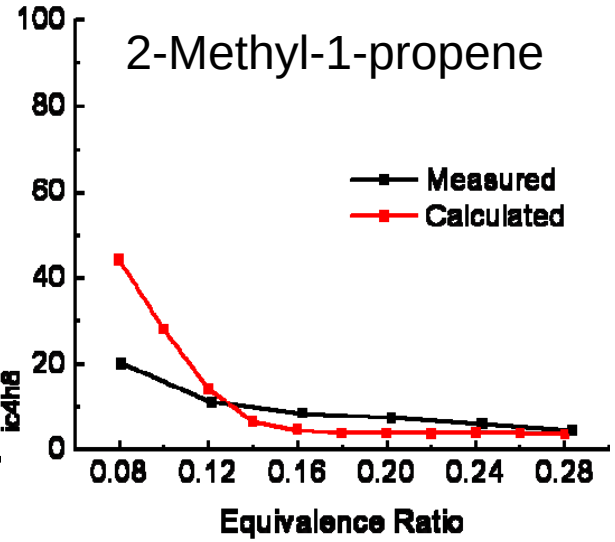
# Our model can predict pressure with good accuracy for a broad range of experimental conditions ($0.08 \leq \phi \leq 0.28$)

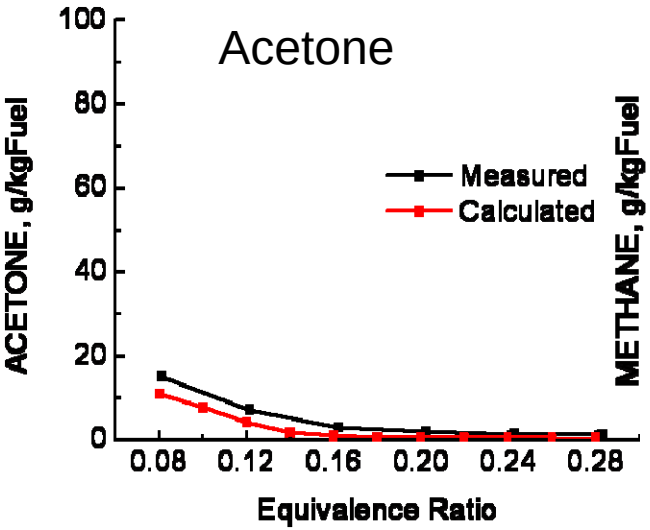


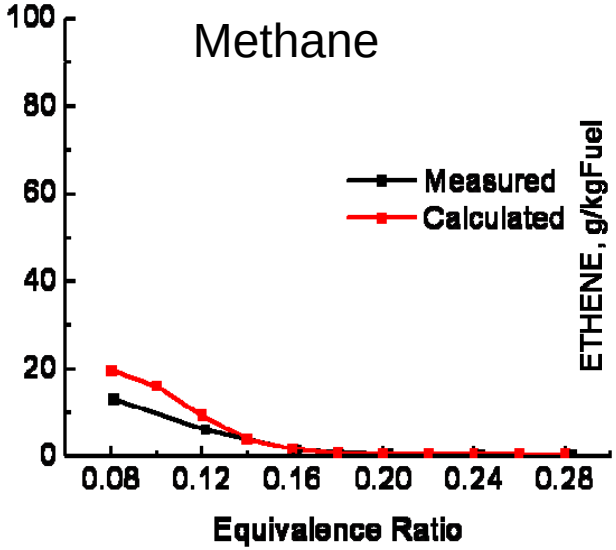
# The model also generates accurate predictions of multiple intermediate hydrocarbon species

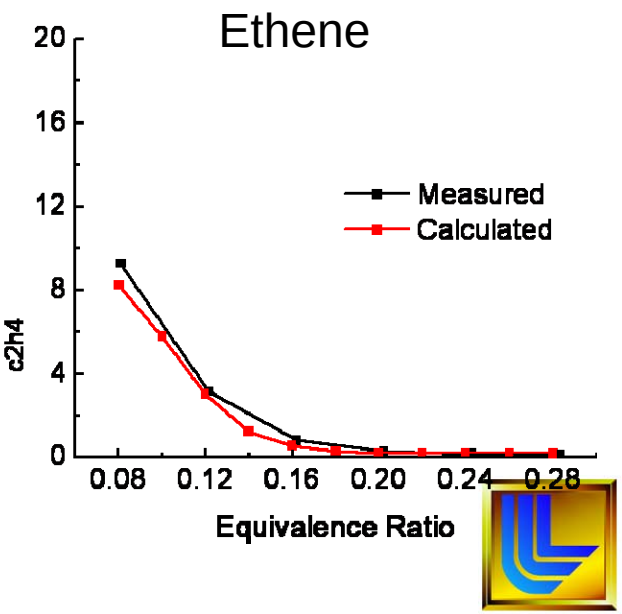


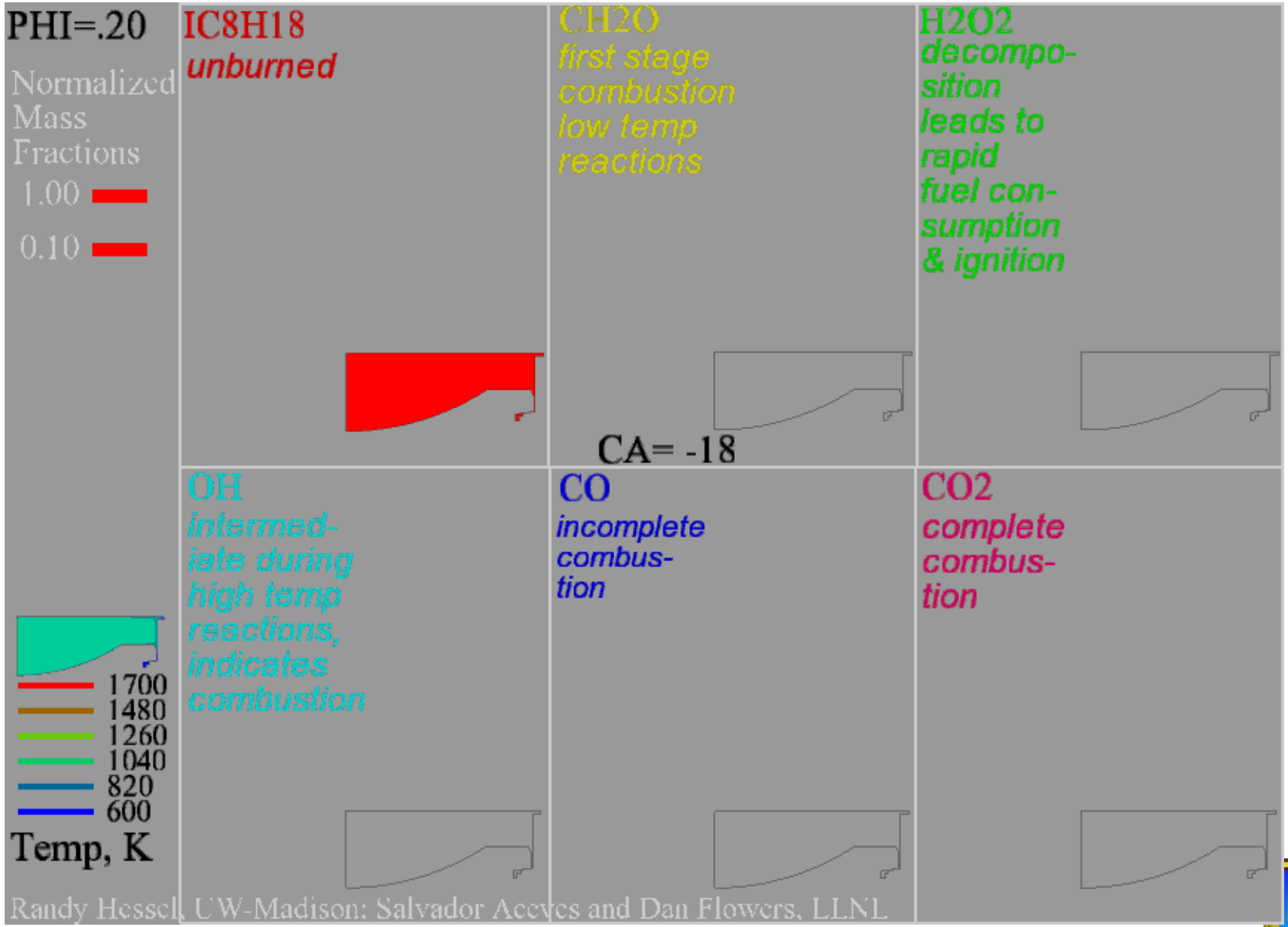



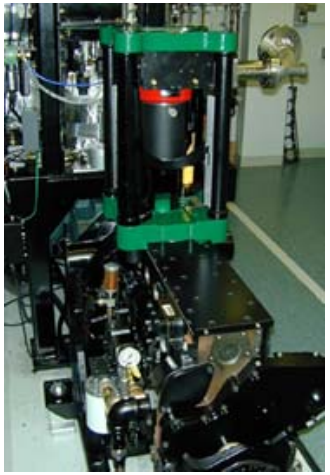



# Our model calculates the location in the combustion chamber where hydrocarbon species are produced

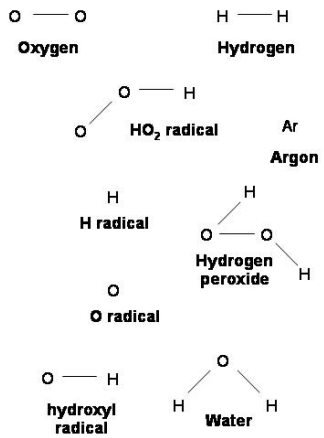


# Unprecedented prediction of specific exhaust species possible due to synergies in collaborator's capabilities

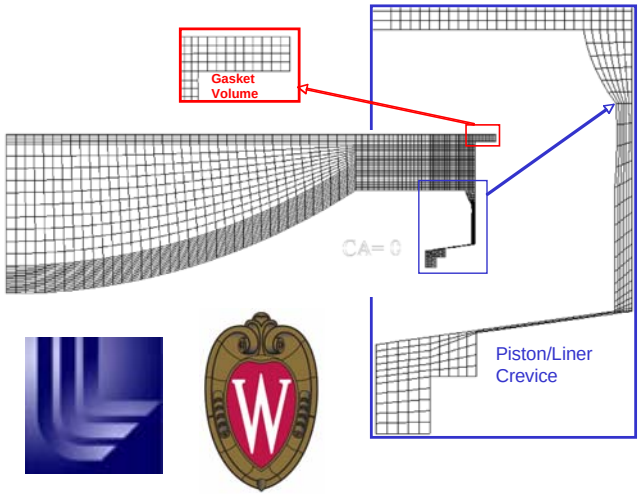


High quality HCCI engine experiments

Analytical chemistry for detailed exhaust speciation

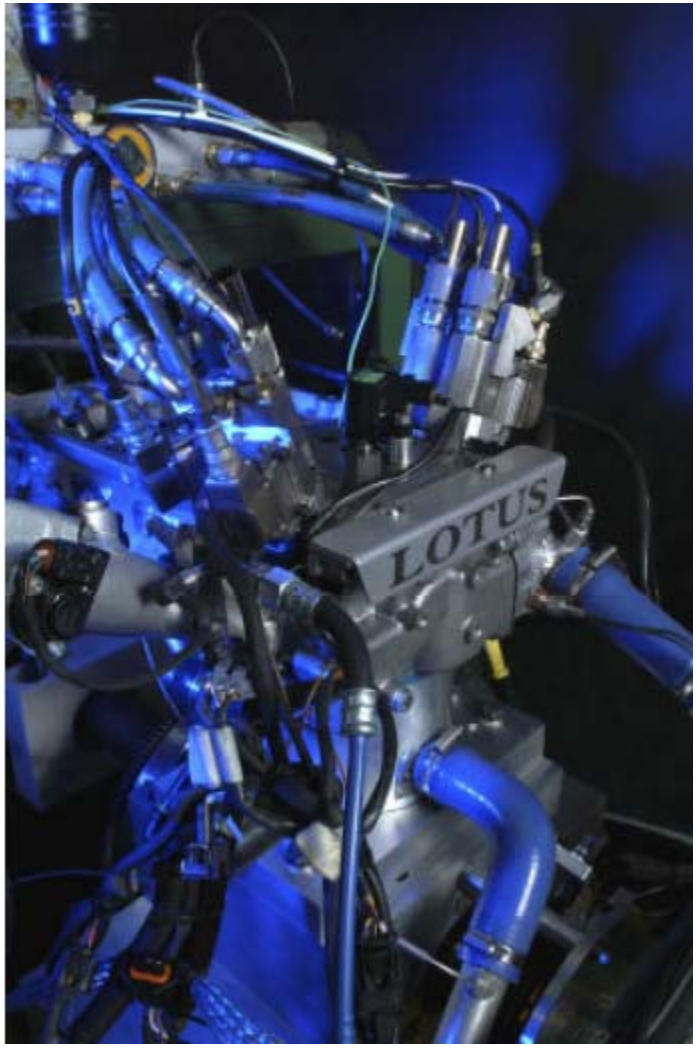



Extensively validated chemical kinetic models

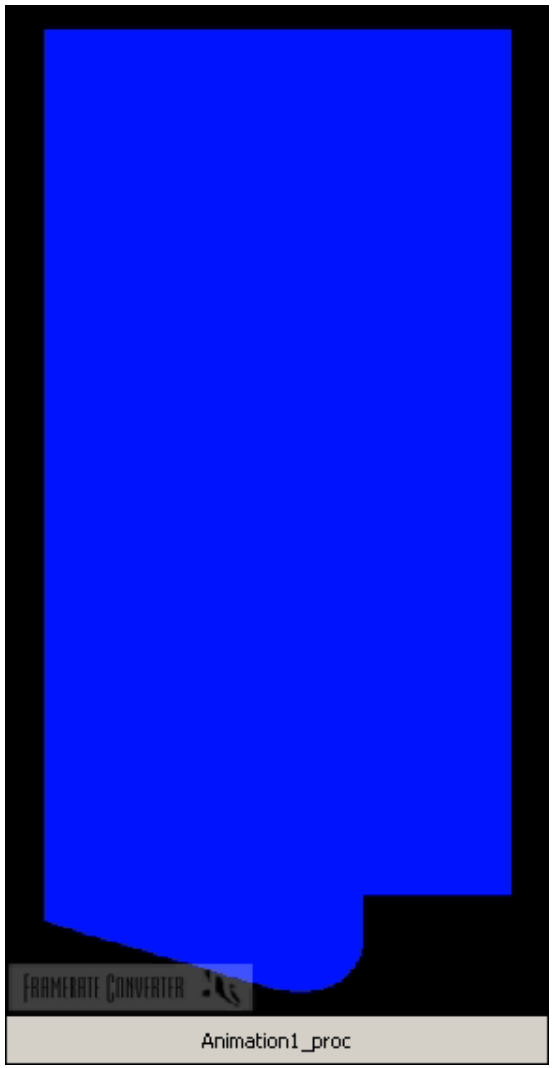



High fidelity engine analysis

# Much interest exists on Premixed Charge Compression Ignition (PCCI) engines for high load and improved combustion control




PCCI through high EGR that does not mix well with fresh charge (VVT CAI)

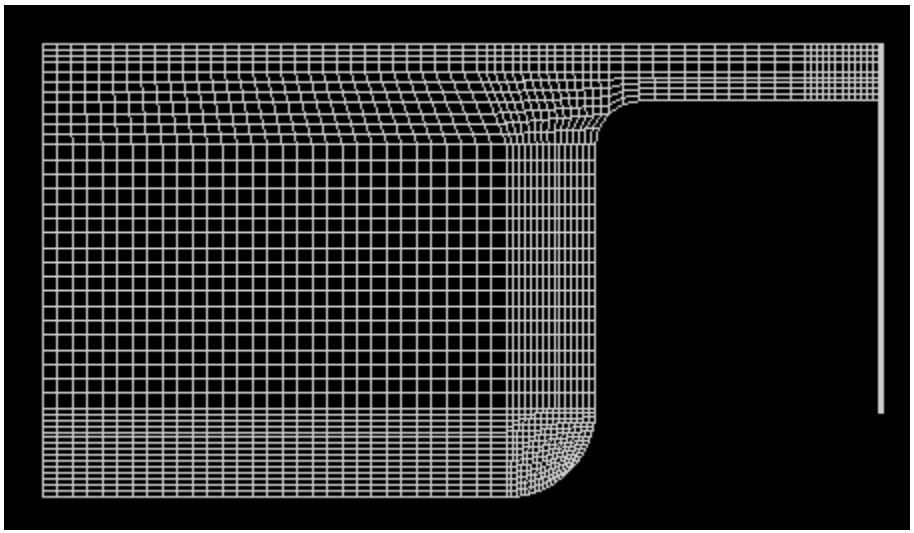


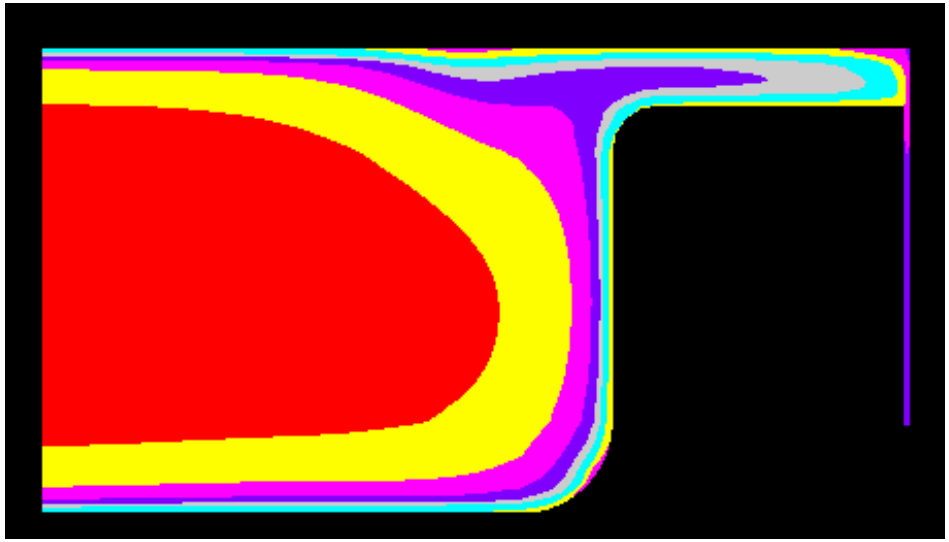

PCCI through early direct injection

## Can we extend our sequential fluid mechanics-chemical kinetics model to model PCCI combustion?

High resolution CFD simulation ($10^5$ cells)

Lower resolution chemical kinetics discretization (10-100 zones)



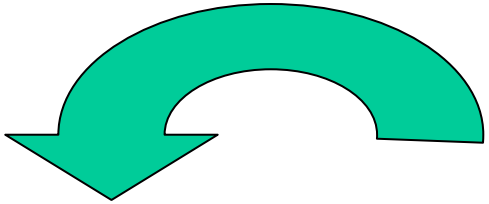


Fluid mechanics sets the temperature distribution where autoignition occurs

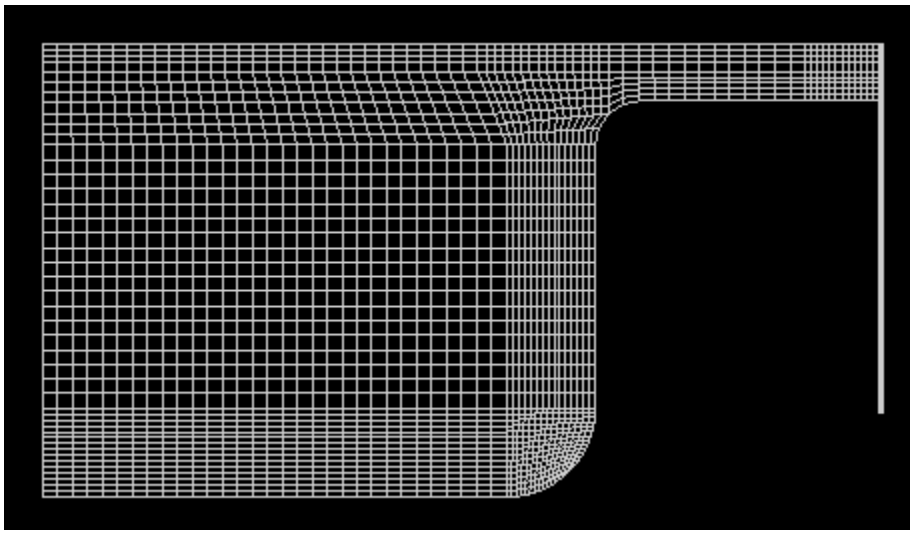
Combustion is very fast and therefore can be analyzed without considering mixing or turbulence

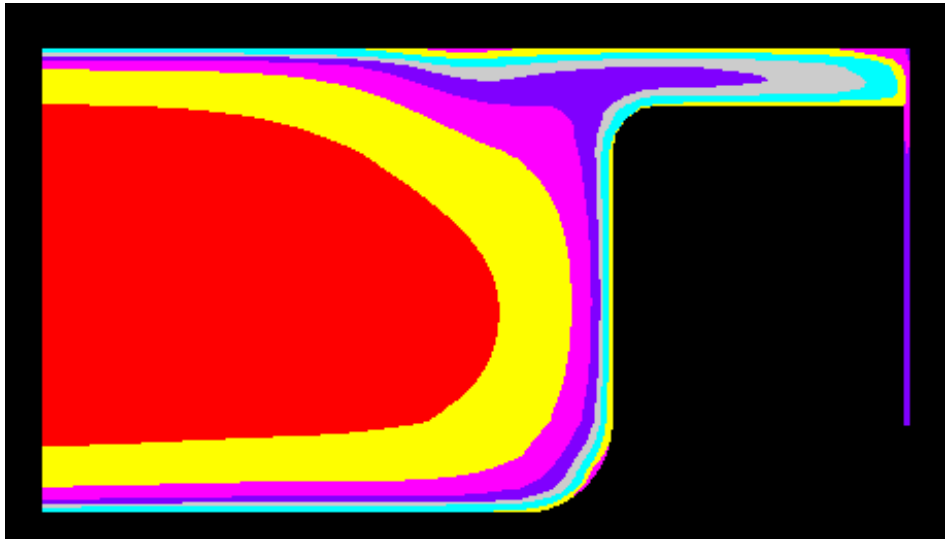
# We can try analyzing PCCI by doing a two-directional mapping, from KIVA to CHEMKIN and from CHEMKIN back to KIVA

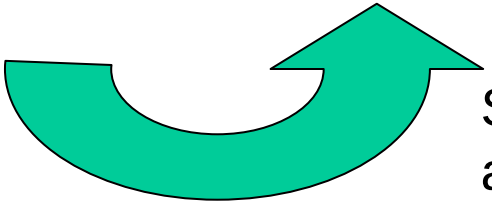
High resolution CFD solver handles mixing, advection and diffusion (~100k cells)



Chemistry handled by multi-zone detailed kinetics solver (10-100 zones)

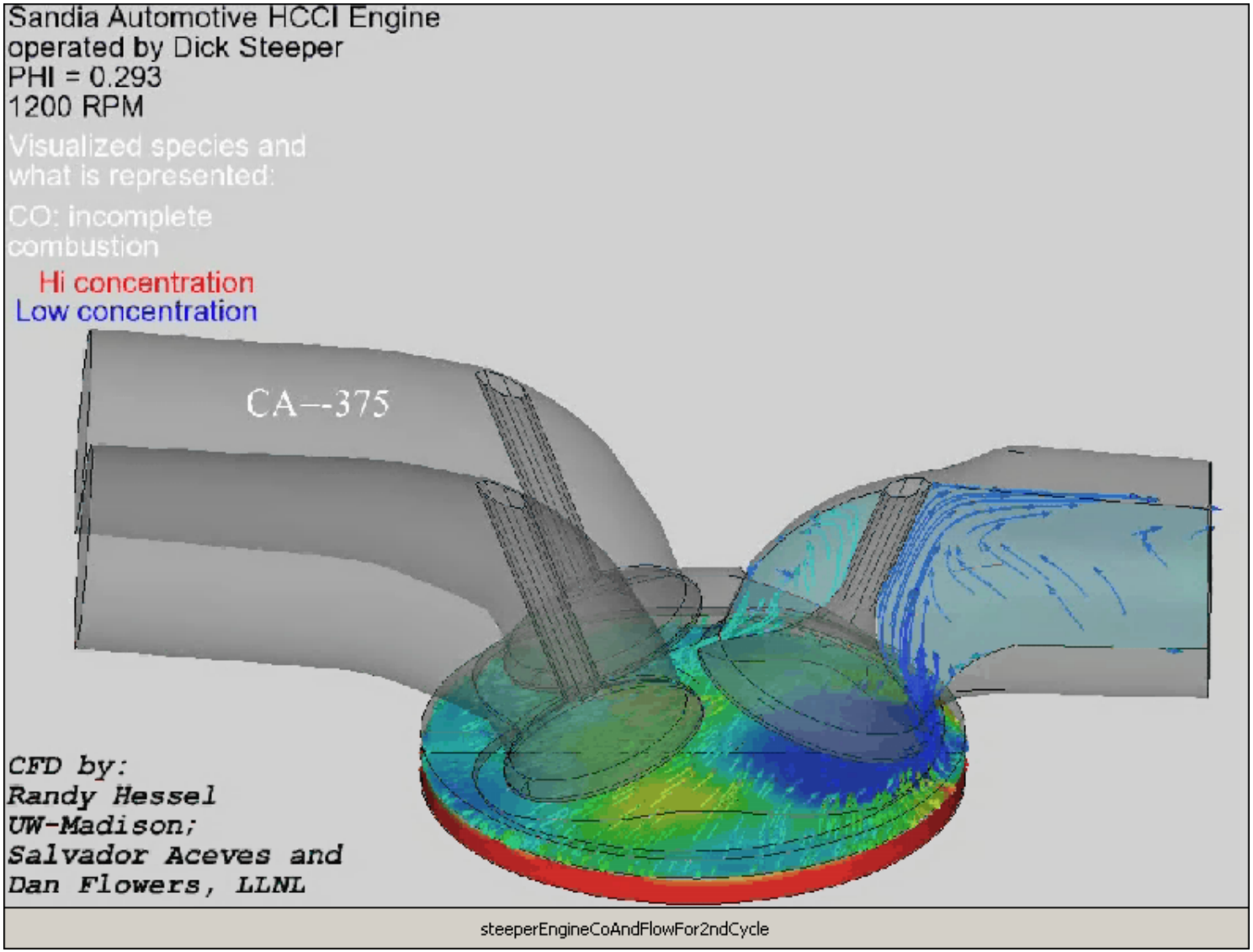






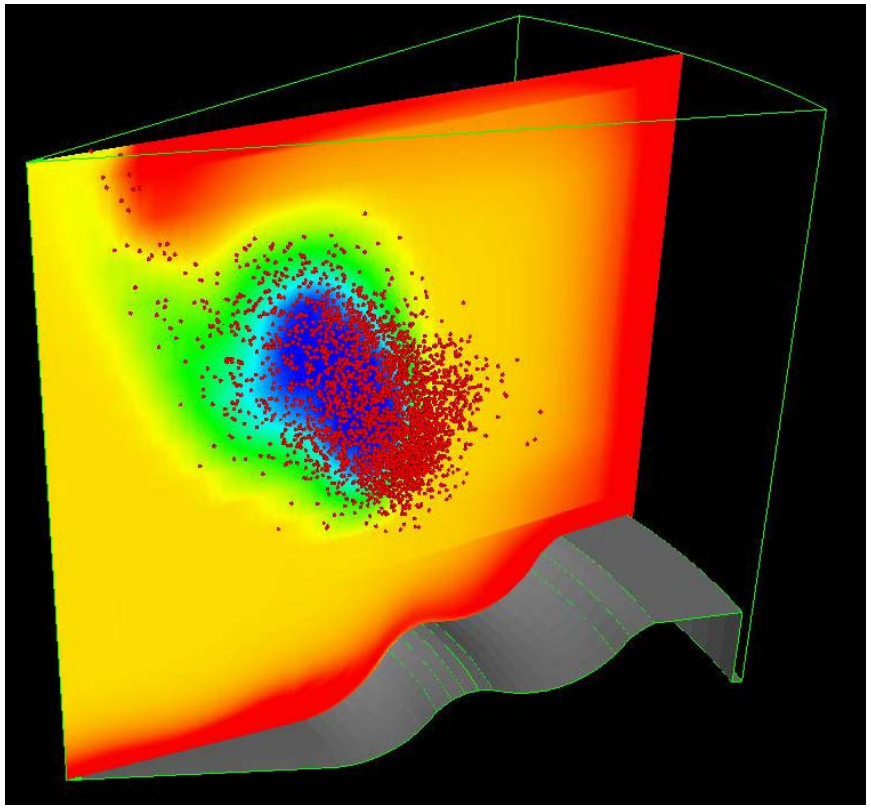
Solutions are mapped back and forth between solvers throughout the cycle

# We are working on applying and validating KIVA-MZ-MPI to a direct injected engine

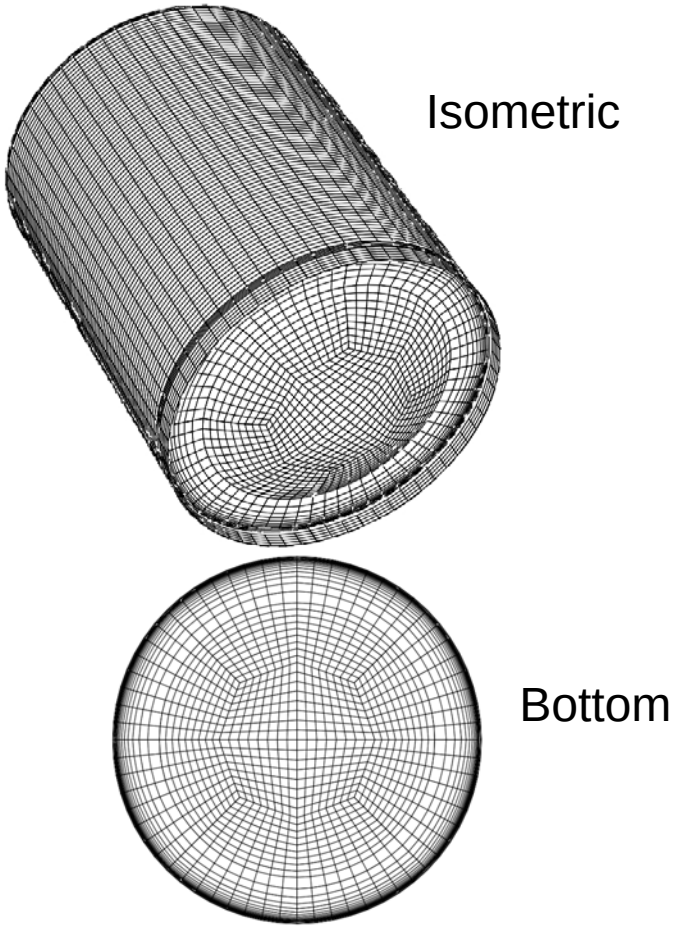



**Direct injected engine at Sandia Livermore (Steeper)**

# We are working on Diesel PCCI Modeling (International) and Kiva4-MZ development (Los Alamos)



**Kiva3v-MZ-MPI investigation of ITEC Early DI PCCI**




**Massively Parallel KIVA4 3D Grid for Sandia HCCI engine**

KIVA4-Unstructured Grids greatly help mesh quality for engine geometries